

Cover Page – Proposal Summary

The first page of the proposal shall be the completed Proposal Summary Form included in Appendix A. If the project requires extraordinary support beyond the normal support for a Z experiment, such requirements and the source of such support must be identified.

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Narrative Cover Page 1

Name and Type of organization: The University of Texas at Austin

Project Title: Understanding the Physics and Chemistry of Iron Alloys relevant to the Conditions of Planetary Cores

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Project Objectives:

Recent research results by the deep-Earth geoscience and astronomy communities have revealed a wealth of interesting and outstanding fundamental science questions about the interiors of terrestrial planets and exoplanets including the origin of the magnetic field in the iron core and its impact on the evolution of life, the alloying of light elements on physics and chemistry of the planet's dynamic processes, and the discovery of super-rotation and heterogeneous behavior of the inner core. Resolving these questions requires a first-hand experimental database at relevant pressure-temperature (P-T) conditions, but is technically challenging using static diamond anvil cell (DAC) and dynamic shock wave efforts alone, due to their limited P-T conditions and analytical capabilities. However, the recent advent of new capabilities of Sandia's Z-Machine, coupled with our recent developments in in-situ ellipsometry at the UT Austin and Sandia National Laboratory and first-principles calculations and geodynamic modelling capabilities at UC Berkeley, motivates the joint collaborative effort presented here.

In this collaborative research, we will use the capabilities of Sandia's Z-Machine to investigate the elastic, thermal transport and melting properties of material relevant to both Earth and exoplanets at their relative P-T conditions. Our long-term research goal is to better understand the physics and dynamics of planetary interiors through interdisciplinary collaborations between physicists, mineral physicists, theorists, geodynamicists, and astrophysicists. The conditions in the Earth and super-Earth can range up to ~ 300 -500 GPa and ~ 5000 -8000 K. We will couple these experiments with a unique set of diagnostics, to include a new ellipsometry capability, in order to sensitively measure conductivity of these materials, and phase changes, including melting. Specifically, the newly demonstrated capability of Z to shock materials to a given P-T along the Hugoniot, and then to apply a pressure ramp taking the material along an isentrope, provides a unique opportunity to obtain P-T conditions not accessible by traditional DAC technology, or through shocks simply along the Hugoniot. Our physics team will perform experiments and analyze results to determine the physics underlying iron alloys as high-energy planetary impactors, classic transition metal alloys, and iron-bearing periclase relevant to the interiors of rocky planets, including exoplanets. The experimental results so analyzed will provide data that our collaborative team of mineral physicists, geodynamics, seismologists, and astrophysicists will apply toward obtaining a fundamental understanding of the physical and chemical states of the terrestrial planets and exoplanets, including their chemical compositions, thermal transport behavior, origin of magnetic fields, and dynamic evolution of the planet.

The material of emphasis in this proposal is iron, the most abundant transition metal in the solar system and in the universe. Due to its natural abundance and unique physical and mechanical properties, especially as alloys in extreme conditions, it has been commonly used as a high-impact material. The partially-filled $3d$ electronic orbitals in iron alloys gives rise to its rich physical and chemical properties with variable electronic, magnetic, structural states. The addition of light elements, such as Si, C, and S in particular, can significantly alter the mechanical and thermodynamic states as well as structures and phase diagrams at extreme conditions. These properties could give rise to the complex seismic heterogeneous signatures of the inner core that have yet to be understood. These candidate light elements are believed to account for 10 wt% of the core constitution that co-exists with iron with ~ 5 wt% Ni, and can significantly affect our understanding of the chemical and dynamic models of the planet. Specifically, the alloying of a major light element can drastically affect the melting temperature (melting point depression) and thermal conductivity of iron at high P-T. It is thus conceivable that the physics of the iron alloys at extreme environments of a high-impactor and planets' cores can be quite different from that under ambient conditions. However, much of our current understanding on the physics and chemistry of candidate iron alloys at planetary core conditions heavily relies on extrapolation of relatively low P-T results (e.g., Birch's Law, Wiedemann-Franz Law) and theoretical predictions. Specifically, the thermal transport properties and melting curves of iron alloys are critically needed to evaluate the current state of geodynamo, the origin of the magnetic field, the thermal evolution of the planet, and the potential existence of a magnetic field in the recently discovered super-Earth. Experimental results from the proposed experiments using the Z-Machine thus provides a unique opportunity to closely examine the physics of iron alloys at unexplored P-T and stress-strain rate regimes that are of great national security interests and of significance in condensed matter physics and planetary science.

Merit Review Criterion Discussion:

Scientific and technical soundness, feasibility of accomplishing the objective

Z Shock-Ramp Experiments for Material and Electronic Measurements

In mid-July, 2015, a seminal shot was performed on iron, demonstrating for the first time that true Earth-core conditions could be controllably achieved using shock-ramp shots on Z. We are working with Dr. Chris Seagle of the Sandia National Laboratories, who designed this experiment, on a set of pulse shapes for our experiments. His Z shot achieved a stress on the impact-side of the target from the shock of approximately 280 GPa at the peak pressure, which was then ramped up to a peak stress of 380 GPa. The release on the back-side of the target into the LiF window was 160 GPa after the shock, and ramped up to slightly over 280 GPa. Our investigations relevant to the Earth's core, will require a slightly higher pressure of approximately 300 GPa at the Fe/LiF interface, but is less than the estimated peak stress limit of the current Z machine of about 400 GPa [personal conversation with Dr. Chris Seagle]. Possible improvements can be made by increasing the magnitude of the initial shock such that the LiF release is closer to the limit of transmissibility. This prior accomplishment of attaining Earth's core conditions on Z on iron greatly mitigates the risk of this proposal to achieve desired P-T.

A figure showing of the current capabilities of the Z platform to drive iron is shown in **Fig 1**, overlaid with representative geotherms, and iron Hugoniot and melt lines. The highest available conditions in P-T parameter space on Z is current-limited. In shock-ramp experiments the available energy is divided between shocking the material, and the ensuing ramp portion of the drive. Our shots will explore the material properties along quasi-isentropes at a variety of temperatures, and we will use a range of current drives that have greater than a 300 ns rise time, to avoid generating a shock in the sample.

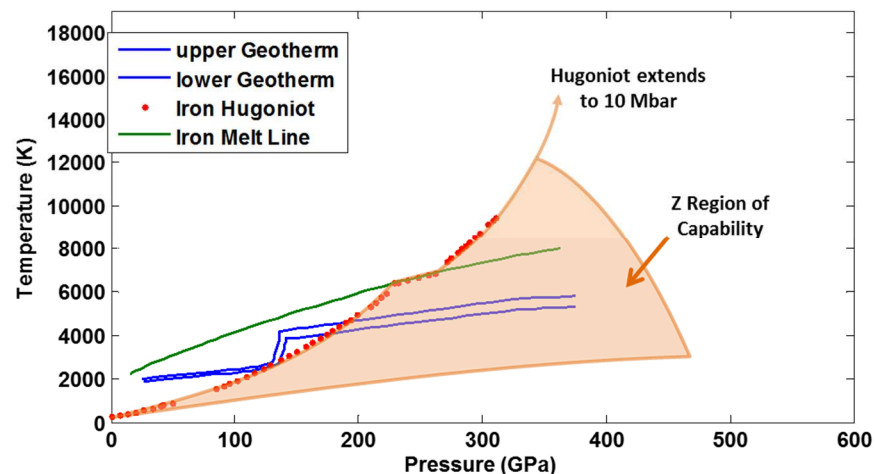


Figure 1: This diagram shows relevant Geotherm lines as well as the iron Hugoniot and melt lines in relation to a rough indication of the current capabilities of the Z Machine as a shaded region. The limit of Z-capability at the lowest temperatures is achieved through pure ramp operation, whereas the highest regions follow the Hugoniot for iron. We note that it is possible to probe the release state that sends this region along isentropes to the “left” of the Hugoniot (lower pressure region).

Our detailed current drive temporal shapes will be developed in the same way that Dr. Seagle did, which involves simulating material response using the LASLO code, a one-dimensional magneto-hydrodynamics code that solves the one dimensional mass, momentum, and energy conservation equations in Lagrangian form. These simulations are required in order to drive the target material to relevant P-T, even at the target/window interface where optical measurements will be performed, while avoiding pressures profiles that cause a loss of transparency in the window material, either during the initial shock (~2 Mbar for a LiF window), and during the ramp phase for a window of extended depth.

Sean Grant, the UT student currently involved in this research, is currently at Sandia full time, and has already developed a proficiency in performing such simulation work to design targets (see Section: Target Design for details). In all stages of our experimental development we are working with Sandia material scientists to determine the exact machine and target configuration.

Nearly all P-V diagrams of shock-ramp experiments in the literature show the target being driven to a point on the Hugoniot, and then following a quasi-isentrope as it is ramped to higher pressures. The isentropic path is indicated by arrows pointing to the right of the Hugoniot in **Fig. 2**. These experiments thereby measure material conditions at lower temperatures than for a give pressure on the Hugoniot, attractive for measurements of the materials at conditions of the Earth's interior. It is worth noting that the shape of these paths follow closely the melt curve, such that these measurements are also advantageous in exploring the melt line at points off the Hugoniot (**Fig. 2**).

However, this set of paths stemming from the Hugoniot represents the material undergoing a shock, then a ramp stage directly, and not one that undergoes the release experienced by the side of the target opposite the impacted side. This opposite side of the target is in contact with a lower impedance window such that there is reflection of a rarefaction wave from the target/window surface. Therefore, at any given time in the material response, a different P-T is achieved before the ramp is applied. The condition of the impacted surface, which coincides with the paths drawn in **Fig. 2**, is indeed determined by the shock-ramp experiments at Sandia Z machine, as the sample density history is determined throughout its entire depth and for the entire history of the experiment [Seagle et al., 2013]. Therefore the right-going paths in **Fig. 2** are relevant to a significant amount of obtained data. However, our optical diagnostic will measure only the surface in contact with a partially impedance-matching window. At this interface the material experiences shock release into the window, which produces a significant pressure drop, such that the starting condition at the sample/window interface at the beginning of the ramp will be to a significantly lower pressure, and slightly lower temperature, somewhere to the “left” of the Hugoniot in **Fig. 2**. The exact trajectory of this release and the following ramp will have to be modelled, but is affected when encountering the melt curve in either release [Tan and Ahrens, 1990] or in the ramp stage. The general area of possible exploration to the left of the Hugoniot is shown in the *Fig. 2* as a blue area, which involves a significant extent of the iron melt line.

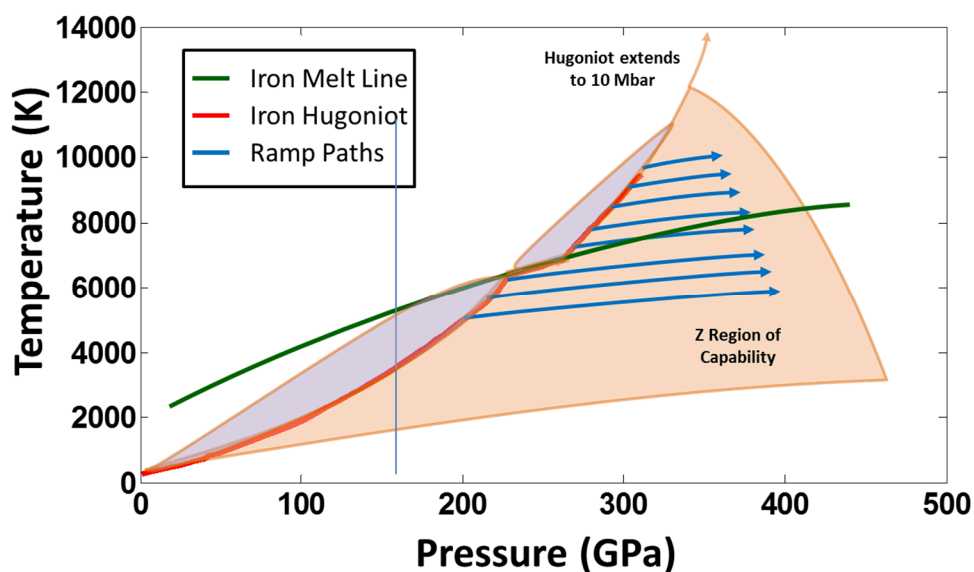


Figure 2: This diagram indicates a range of possible ramp trajectories off the iron Hugoniot achievable on the Z Machine as well as their relation to the iron melt line. During such experiments the sample will progress along this ramp trajectory as a function of time.

Ellipsometry Development

We are proposing a unique diagnostic implementation for these Z shots, which we have developed in conjunction with Sandia materials scientists over the past few years, and has been the main project of Sean Grant, a UT physics graduate student. This is an ellipsometer, initially of Dr. Aaron Bernstein's design at UT, built at Sandia by UT PhD student Sean Grant along with on-site advising by Dr. Tom Ao. Dr. Dan Dolan, Dr. Chris Seagle, and Dr. Jean-Paul Davis. Our ellipsometer has been developed from the beginning with an effort toward reducing issues associated with electrical signal noise that plagues large high energy density machines, and for optimal implementation using the current Z diagnostic infrastructure. This UT/Sandia collaboration will be ongoing for the duration of this project (please see relevant support letters from Dr. Seagle and Dr. Benage), which supports Sean as a PhD student intern, provides valuable material, equipment, and computing resources, as well as funding the construction of versions of the ellipsometer (see Section [1]).

Ellipsometry on Z is a great advance as it introduces a new capability to sensitively measure material conductivity and material changes, such as phase changes through time-resolved optical measurement of that materials' electronic properties (see Section [1]). Ellipsometry measures changes in the phase and amplitude of orthogonal polarization directions of light that results from that light's reflection off a sample surface at an oblique angle. These changes are sensitive to the electronic properties of the material, such as electrical and thermal conductivity, and can be used to directly determine the complex dielectric constant for the wavelength of the probing beam. Current theoretical estimates of the thermal conductivity vary by a factor of three so any measurements will be extremely useful [Pozzo et al., 2012, 2013; Zhang et al., 2015]. The physics team at UT Austin will perform ellipsometry measurements to determine conductivity. The complex dielectric constant complements well data obtained by current Z diagnostics, including point Doppler velocimetry (PDV), streaked visible spectroscopy (SVS), reflectance, and velocity system interferometer for any reflector (VISAR). Our measurements will employ multiple ellipsometers, optimally arranged to interrogate multiple samples within the available diagnostic space of the Z machine.

We have fielded ellipsometry on experiments using the gas gun at the DICE facility at Sandia, which is capable of launching projectiles up to 300 m/s. The diagnostic is schematically illustrated in **Fig. 3**. Fiber optics relay the optical signal from the ellipsometer well away from the violence of the experiment, and out of the vacuum chamber for recording on a fast oscilloscope. The ellipsometer apparatus must be aligned and calibrated in-situ before the shot, and must be completely replaced after each shot. In order to optimize use on Z, this design has considered from the beginning the existing diagnostic infrastructure on Z, including the use of fibers and the wavelength of the near infra-red probe. The dynamic experiments we have so far conducted at the DICE facility at Sandia have demonstrated that our design is feasible in the extreme conditions of dynamic materials experiments over their entire lifetime (microseconds).

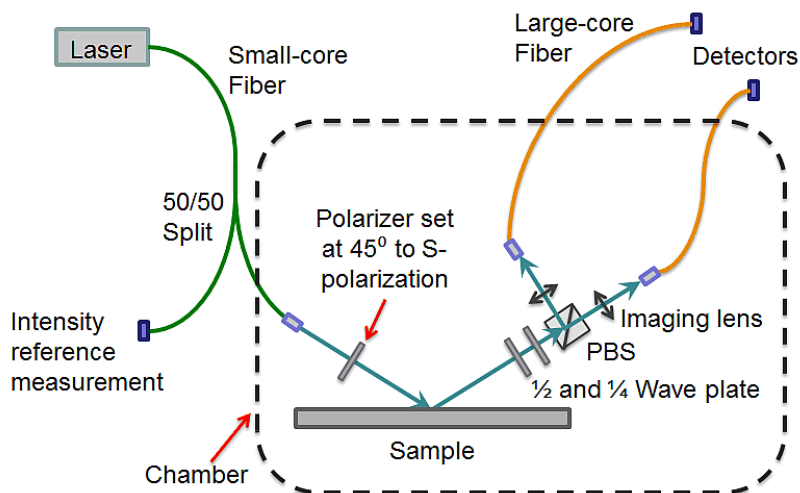


Figure 3: Schematics of the ellipsometry design. The dashed line represents the boundary of the vacuum chamber enclosing the experimental sample and ellipsometer. In the perspective of this figure, the sample is impacted from below.

The ellipsometer operating principle does not vary much from previous devices. In fact, it shares one feature which was commonly used long ago on ellipsometers, but is rarely found on newer ones: we use a “compensator” in the form of a quarter-wave plate after the sample. The compensator was used primarily on manually operated ellipsometers to produce a “null” value as part of their measurement. In our case, we use the quarter-wave plate to evenly distribute the signal among the two receiving fibers, vital for determining the complex dielectric constant from our signal. The quarter-wave plate accomplishes this by transforming the instrument from one that measures changes of a linearly polarized probe to one that measures changes to a circularly polarized one.

We analyze our data using numerical fitting/solving based on matrix equations built up using the Jones matrix formalism. These equations can be used to fit/solve for unknowns, often the complex dielectric value of the sample at the probe wavelength. Results from our ellipsometer on static samples are illustrative as they show an interesting feature: that the complex dielectric constant gives information complementing measurements of reflectivity alone. In the **Fig. 4**, we show data obtained using our ellipsometer in comparison to those of a commercial ellipsometer operating at the same wavelength. We see excellent agreement between measurements from our ellipsometer and those of commercial unit. These measurements were all made on the same sample, but when we compare the result of this pure gold sample to measurements found in the literature, we see an interesting feature: that they all lie roughly along a contour line that represents constant reflectivity (**Fig. 4**). In fact, the total spread in reflectivity of the measurements in literature is []%. The explanation for the difference in measurements of the dielectric constant for what are pure samples of gold may lie in the very minute differences of impurities. It is more likely, however, that the difference lies in the technique used to deposit the gold on the substrate. This sensitivity to morphological features is a demonstration of the utility of the ellipsometer to detect material changes occurring during a phase change, and which may be missed by a reflectivity measurement alone.

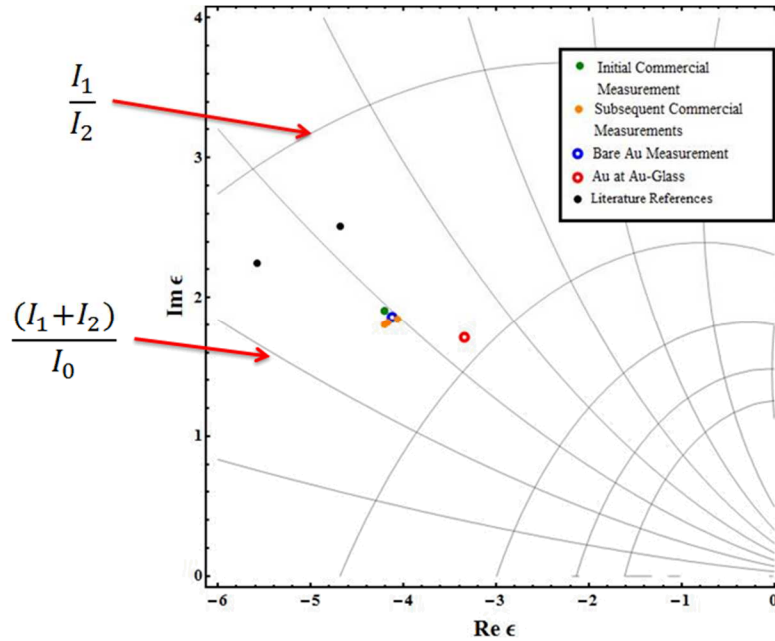


Figure 4. Preliminary reflectivity result of pure-gold sample using the ellipsometer design. These dielectric constant results are compared with literature values.

Once the complex dielectric constant, ϵ , is obtained, they relate directly to the complex conductivity by $\sigma = -i\omega\epsilon/4\pi$, where ω is the laser frequency. For materials with a preponderance of free electrons (metals), we can then, by the Wiedemann-Franz law, relate electrical conductivity to thermal conductivity. This law is generally accepted to apply to Earth-core materials (iron and iron alloys), especially at the high temperatures of interest here. Indications are that the Lorenz parameter is nearly a constant along adiabats for different alloys [Pozzo 2013]. Further, theoretical calculations for at least the real part of the electrical conductivity of iron over a range of wavelengths demonstrates a fairly flat over the first ~ 2 eV, indication that our measured value at 1550 nm (0.8 eV) will be representative of the DC value. However, the predictions of Pozzo et al. [2012, 2013] suggest the thermal conductivity of iron should be very high (possibly too high to permit thermal convection). If the calculations by Zhang et al. [2015] are correct, the effects of electron-electron scattering at high temperature would moderate these effects. By reaching higher temperature using Z Machine, it may be possible to increase the magnitude of the effect above the level of detection. Furthermore, it also remains to be tested experimentally though as to how the alloying of a light element such as Si can affect the electrical and thermal conductivity of liquid iron at the P-T conditions of the Earth's core and exoplanets.

We ran three experiments on the DICE gas gun over the past year at Sandia National Laboratories to test the ellipsometry diagnostic. These experiments consisted of gold coated BK7 samples. The BK7 was shocked to about 1.4 GPa. These experiments tested feasibility of the ellipsometer for use in dynamic experiments, as well as its probing of both the gold's dielectric constant and the shock-induced birefringence in the BK7. This series of experiments proved also that the ellipsometry diagnostic is easily adaptable to different probe wavelengths (1550 and 1310 nm were both tested in this case, but other wavelengths could easily be used given laser light). **Fig. 5** shows the device as constructed for these experiments. It uses a commercially available optical frame construction and mounting system for robust and compact operation.

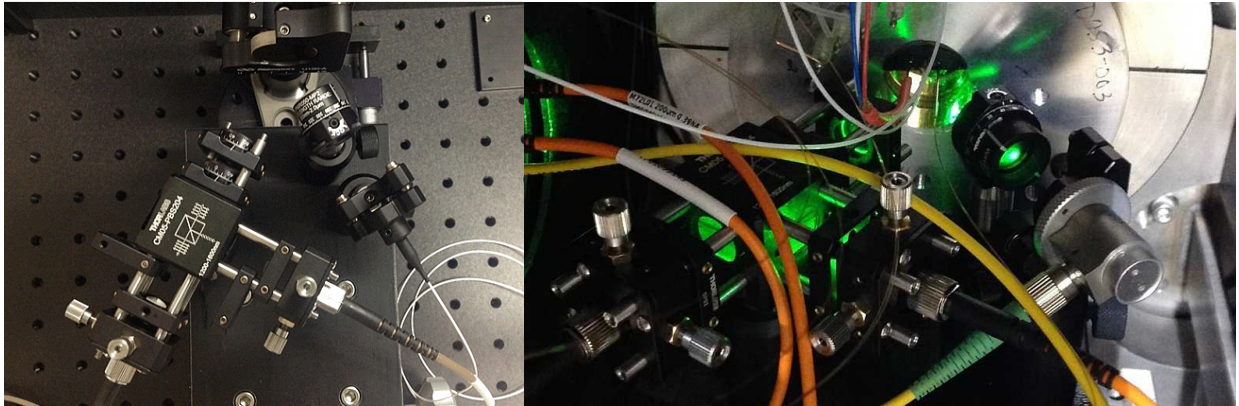


Figure 5. Left: Assembly of the ellipsometer with probe beam delivery and collection fiber optics. Construction uses a “cage” framing and mounting system for rigidity, convenience, and compact design. Right: Ellipsometer assembled and aligned with probe beam present, for use on the DICE gas gun, before a shot.

The three experiments performed at the DICE facility gas gun used 12 mm thick, 1 inch diameter quartz flyers impacting a 5 mm thick, 1 inch diameter BK7 substrate with a 300 nm gold coating on the impactor side. The quartz had an impact velocity of 200 m/s, yielding a shock pressure of 1.44 GPa. As **Figure 6a** shows, the ellipsometry diagnostic was incident on the backside of the sample, looking through the BK7 and reflecting off the gold coating, at an incident angle of 30 degrees.

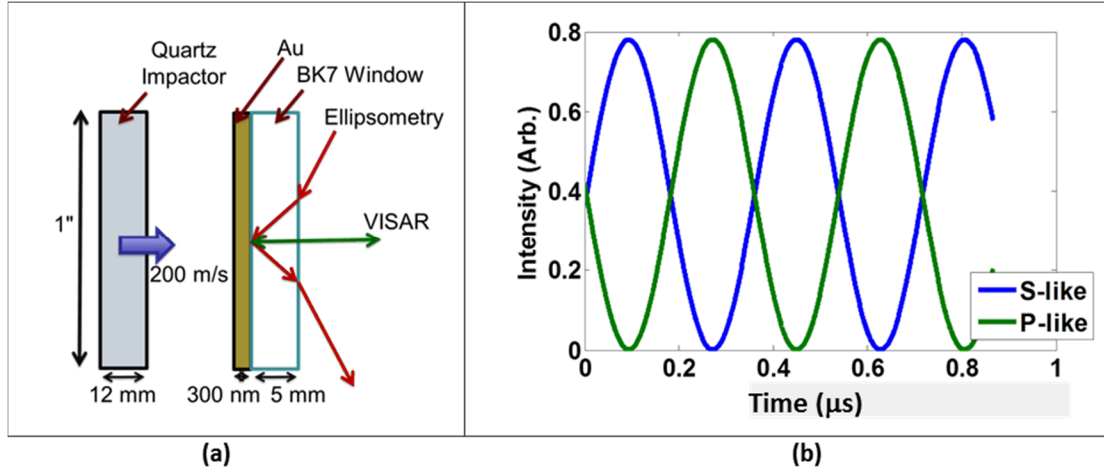


FIGURE 6 . (a) A schematic of our experimental layout. A quartz flier impacts our sample, a BK7 window with a 300 nm gold coating. (b) Modeled signal outputs for this experimental configuration showing the effect of window birefringence.

Using a Jones matrix formalism for tracking polarization propagation we model the anticipated signals from an experiment. In this case, a growing birefringent layer in the BK7 window due to the elastic, uniaxial compression causes a phase shift to steadily accumulate between the two independent polarization axes with time. This phase accumulation manifests itself as a sinusoidal behavior in the signal traces, with an idealized signal of this shown in **Figure 6b**.

All three shots produced data similar to that shown in **Figure 7**. Our experimental data resembles the modeled results well; at shock impact there was an onset of sinusoidal behavior as the shock propagates through the BK7 window, generating a growing birefringent layer. As a testimony to the cleanliness of the results of this experiment, it is seen that after shock breakout (at about $0.75 \mu\text{sec}$) the signal demonstrates the reflection of the rarefaction wave from the free surface of the window, and we see it effectively removing the birefringent layer as it propagates back through the window towards the gold surface. This interaction is partly because the shock pressure was low enough that the window experienced a totally elastic compression, and thus the deformation is reversible.

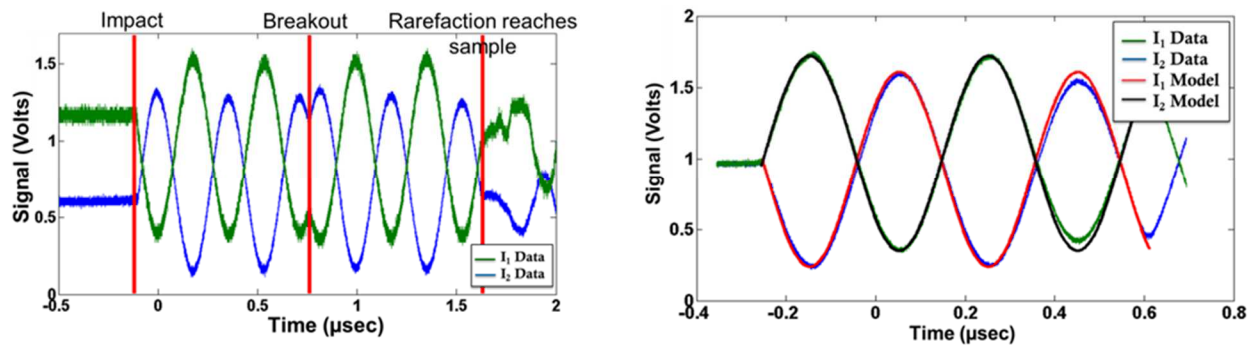


Figure 7. Left: Experimental data with red lines indicating the point in time of the reflection of a rarefaction wave from the free surface of the compressed dielectric (and birefringent) window. Right: Modeled signal outputs fit to the data.

We are able to fit our model to the data in order to pull out the strength of the birefringence in the BK7; the strength of the birefringence is one of the main contributions to the period of the oscillations in the data. Using as input parameters the shock speed in the BK7, the ambient index of the BK7 (1.5007),

and the ambient dielectric of the gold, we find the extraordinary index of the BK7 to be 1.50391 ($\Delta n = .0321$).

We also zoom in on the data at impact time to look for changes in the signal caused by a change in the gold's dielectric (**Fig. 8a**). There is an increase in both signal traces over a period of about 20 ns before the sinusoidal behavior of the birefringence takes over. Taking this data we can analyze each point in time to derive a plot of the gold's dielectric as a function of time (**Fig. 8b**). Here we have done the analysis with the assumption that the birefringent layer has not yet begun to grow. This analysis shows a decrease in both the real and imaginary parts of the gold's dielectric contributing to this increase in reflectivity.

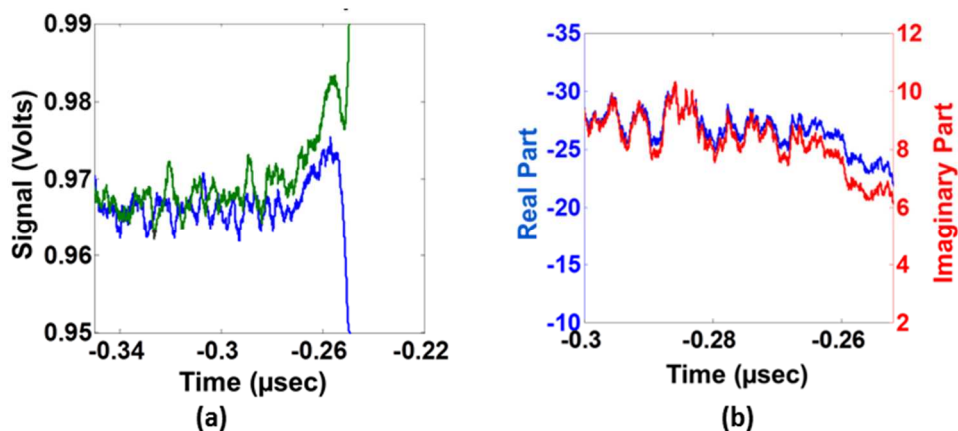


FIGURE 8. (a) The experimental data zoomed in on initial impact. The sharp jump in the signals off the plot is the onset of the sinusoidal behavior. (b) The analysis of the initial time data yielding the real and imaginary parts of the gold's dielectric as a function of time.

The plots in **Figure 8** demonstrate the quality of the data of the ellipsometer in the extreme conditions of dynamic materials. To measure a sample with dielectric properties that vary more greatly over the achievable pressures on DICE, we will measure shocked preheated samples of tin. These targets will consist of a layer of pre-heated tin to 270 K on LiF substrates, and we will compare results between this and a shot taken with an ambient-temperature aluminum impactor. This second sample was hot enough to melt upon impact. Further experiments are scheduled for these test experiments on the STAR facility, which has a gas gun that can accelerate flyers to km/s. The ellipsometer results have been encouraging enough to warrant interest by Sandia researchers to field it in late summer of 2016 (see attached support letter).

Target Design

An important aspect of this proposal is the effort level we will spend on producing appropriate and high quality targets. In these considerations we have been communicating directly with Chris Seagle, Tommy Ao, and Jean-Paul Davis at Sandia. The LiF substrates for our targets can be purchased by vendors, such as Asphera Incorporated, with a clean polished surface. These substrates can then be coated with an iron deposition layer as well as a tantalum capping layer in Tech Area 1 at Sandia – other deposition options are available there as well if needed. The gluing of any extra layers would be done in Tech Area 4 at Sandia. This use of Sandia facilities is not requested in this proposal per se, but is rather an extension of our ongoing collaborative research with Sandia materials science investigators.

While the achievable parameter space on Z is current-limited, as mentioned in the prior subsection (**Figs. 1-2**), the achievable parameter space is also limited by target considerations. Specifically, the transparency of LiF at high pressures depends on its dynamic history; LiF is known to maintain transparency up to 200 GPa [Furnish et al., 1999; Hicks et al., 2003; Rigg et al., 2014] but can retain

transparency to higher pressures if instead it is first shocked to less than 200 GPa, then ramp-loaded. LiF has been shown to be transparent under ramp loading up to 800 GPa [Fratanduono et al., 2011].

In our experiments it will be necessary to ensure that the first shock of a shock-ramp experiment does not exceed the transparency limit. We have considered other materials, such as cryogenic (liquid) noble elements, which similarly exhibit no birefringence, however, these do not match the impedance of the iron target as well. For these reason, we will use LiF for our measurements, which we do not expect to exceed 4 Mbar due to current limitation of Z.

We are currently considering two sample designs for iron (**Fig. 9**). Based on simulations performed by Sandia scientists and Sean Grant, we will down-select the final design from these two designs before the first round of our proposed shots on Z takes place. The first design, shown just below, features a thin-foil deposition about 300 nm thick onto a LiF substrate. To prevent oxidation, a thin layer of titanium (approximately 50 nm thick) will be deposited on top of the iron. Directly impacting this target will likely be flyer plates of either copper or aluminum. This setup would involve very small amounts of iron, which would rapidly (<1 ns) reach pressure conditions associated with impactor hits directly on LiF. This pressure would be lower than would occur on a thick iron sample. The thin iron sample will attain a temperature much closer to the temperature associated with the initial shock onto the iron, which would subsequently decrease adiabatically upon the pressure drop to the LiF layer.

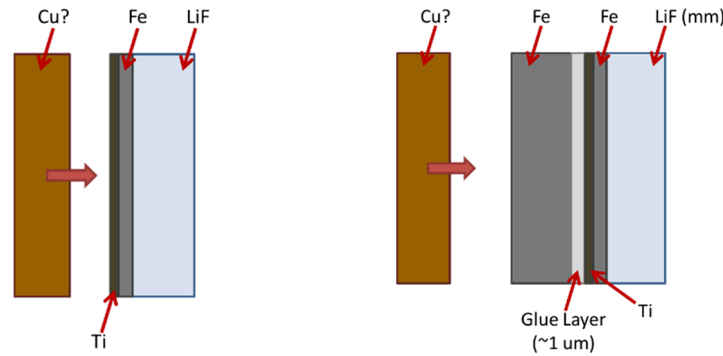


Figure 9. Schematics for the target designs for the proposed experiments on Z.

The second target option has, in addition to the structure of the first option, another thick layer of iron glued to the titanium overcoat layer described above (**Fig. 9** right figure). This target structure is shown below, showing, in order, the layers: LiF, iron sample layer, Ti overcoat layer, glue layer, thick iron. The glue layer would be about ~ 1 μm thick and expected to compress and ramp up very quickly so that the probed iron layer will be much closer to the single release state of iron as it releases into the LiF, providing a higher pressure state to probe. How these targets will interact with shock-ramp compression will be simulated in LASLO Code in order to determine which design to use, and then used to refine the down-selected design. This will take place before the first set of proposed Z shots.

We are additionally considering a variety of iron-alloy materials, which would follow the target designs above, but would require simulation in order to determine the likely P-T conditions achieved. In practice, we will design Z experiments around our explorations of pure iron, and design our alloy and light-element targets to avoid “shock-up” that can occur in sufficiently thick targets even during the ramp-phase that might render our window material opaque. Our preliminary evaluations indicate that the alloys should be easier to achieve the desired conditions, e.g., lower impedance, melting point, and sound speed), but producing alloy targets will be more challenging due to their binary nature.

For materials that are transparent, such as MgO, metallization measurements may be of interest. MgO is also a classic oxide and it's of great interest to investigate its properties in extreme conditions. Furthermore, ferropiclasite ((Mg,Fe)O) is believed to be the second most abundant mineral in the silicate mantle and likely undergoes an electronic spin transition that may give rise to semimetallic behavior [Lin et al., 2005; Lyubutin et al., 2013; Holmström and Stixrude, 2015]. To perform optical measurements, as with our ellipsometer, a reflective coating would be placed on the impact-side of the target. We plan to initially set up the ellipsometer using this reflective surface, and if the shock puts the MgO into a metallic state we will get a signal reflecting off the shock front within the MgO.

Target Configuration and Experimental Layout

The proposal call describes a probable limit of 5 shots per year, so maximizing the value of each shot is of paramount importance. We will use a symmetric (two-sided) strip-line configuration for our experiments, which allows for a maximum of 8 samples. **Figure 10** shows a simplified view of the typical target layout on either sides of the anode/cathode assembly. Samples are typically rectangular with dimensional size of 8x7.3 mm. A metal shroud encloses probe beams that would originate from far left and right of the figure. Adopting a technique currently in use on Z, we will likely use 6 of these samples, and the remaining two will house LiF windows, through which, using VISAR, we will obtain a clean measurement of the “impact time,” important for determining the ensuing dynamics precisely. This layout has become a standard one for shots on Z, and used in Dr. Seagle’s shock-ramp experiments.

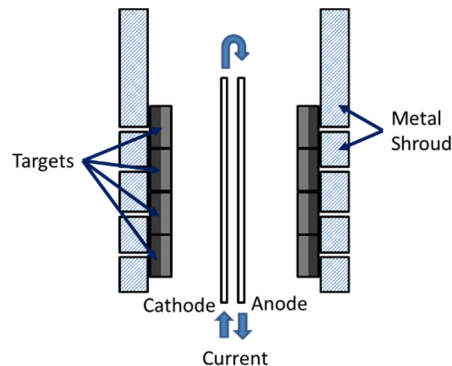


Figure 10. A schematic representation of the dual stripline experimental configuration on Z. The cathode and anode themselves become the flyer plates, moving away from each other to impact the targets. The metal shroud infrastructure defines optical paths and provides a mounting structure for diagnostics.

In consultation with scientists at Z, we have determined that there will be room to field on any one target the ellipsometer simultaneously with either PDV or a SVS/VISAR combination. We plan to do this on a number of samples with the remaining samples diagnosed using a combination of SVS, VISAR, and PDV. This fielding of the standard set diagnostics on a portion of the samples on each shot helps to guarantee data is obtained that can be benchmarked to other measurements using the same diagnostics. The compatibility of various combinations of diagnostics depends on the physical dimensions of the diagnostics and line-of-site access to the target surface. In communications with the collaborating Sandia scientists, we produced a diagnostics compatibility matrix, shown below, which indicates the combinations of diagnostics simultaneously employable on the current Z platform.

	PDV	SVS/VISAR	Reflectance	Ellipsometry
PDV		Yes	Marginal	Yes
SVS/VISAR	Yes		Yes	Yes
Reflectance	Marginal	Yes		No
Ellipsometry	Yes	Yes	No	

An example consideration is the use of PDV on all samples. This will help establish a cross-correlation of results across the samples in a given shot, whether they are measured using ellipsometry (which precludes reflectance) or not. The number of samples upon which ellipsometry will be fielded is a decision that will be made before the first set of proposed shots, and depends on the results of preliminary experiments, including ride-along shots on Z (see Section 1.1).

Sources of Error

Errors that originate with the inherent use of the Z platform are no different in this experiment than in those currently being conducted on Z. This includes thickness of the sample, the velocity of the impactor, the length of the flight gaps, and knowledge of the iron Hugoniot for the initial shock state [Seagle et al., 2013]. The high accuracy of measurements on Z place this platform above those that use lasers or DACs, as measurements are performed on macroscopic samples experiencing a geometrically flat pressure profile.

Errors may arise in the ellipsometry measurements that originate from depolarization on the sample/window surface during the experiment. To some extent the ellipsometry data may be checked by a redundancy in reflectivity information from both the VISAR and reflectance diagnostics. These checks will take place during ride-along shots that are to precede the proposed shots. If depolarization does take place to affect the s and the p polarizations equally, or we know the magnitude of loss for each as a function of time, then this can be accounted to determine the dielectric constant. However, if depolarization affects s and/or p polarization directions independently, we may not be able to reliably determine the electrical properties. In this case, even the “full stokes vector” type technique only considers the degree of polarization, not which term experienced what amount of depolarization. We do have, however, some confidence that this will not be an issue for experiments on macroscopic samples on Z. All indications of such experiments on Z have so far indicated a smooth surface profile, as measured using line-VISAR.

Scientific and technical merit, relevance and prospective contribution to field of research

Relevance to Deep-Earth Interior:

Terrestrial planet interiors are subject to extreme P-T conditions. Pressure ranges from 140 GPa to 360 GPa in the Earth's core, while temperature varies from approximately 4000 K to 6000 K [Dziewonski, 1981; Poirier, 1994]. More extreme conditions are expected in the interiors of the recently discovered exoplanets due to their larger mass [Seager, 2010]. The thermal and chemical states of a metallic core is directly linked to the generation of a planet's magnetic field, how that planet dissipates heat into its silicate mantle to power potential plate tectonics processes, and possibly how a planet can sustain the evolution of life via the shielding of the solar wind by the magnetic field.

Planetary cores are mostly made of iron alloyed with a few percent of nickel, together with certain amounts of light elements that are mostly abundant in the solar system and in chondrites [McDonough and Sun, 1995]. Depending on the formation conditions of the planet, the identity and amount of the light elements can be different. For example, the Martian core is proposed to contain abundant sulfur as the major light element, whereas a number of light elements such as Si, S, and O have been proposed to exist in the Earth's core [Li and Fei, 2003; Vocablo et al., 2003]. The Earth's inner core is believed to contain approximately 4wt% of light elements while the outer core likely contains 8-10wt% light elements. The substitution of light elements in the Fe-Ni alloy in planetary cores can effect a series of physical and chemical properties of iron and thus our understanding of the physics and chemistry of the planetary core. Specifically, the addition of a light element will lower the density and melting point of iron at extreme conditions, and can also change the crystal structure and thermal transport properties of iron [e.g., Lin et al., 2002, 2005, 2009]. During the crystallization of the inner core, latent heat is released and some the light elements are excluded from the solid, providing the primary source of buoyancy for driving convection in the liquid outer core and powering the magnetic field [e.g., Buffett, 2001, 2002, 2009]. On

the other hand, the addition of light elements into iron can lower its thermal conductivity, affecting how heat is transported in the outer core and altering the power available for the geodynamo (Pozzo et al., 2012, 2013). However, these light element alloying effects on the aforementioned properties of iron at the P-T conditions of the Earth's core as well as those of the exoplanets remains mostly unknown experimentally. Specifically, we currently do not know what is the magnitude of the Si alloying effect on the thermal and electrical conductivity across the solid and liquid iron and what is the melting point depression of a light element alloyed with iron in the outer-inner core (OIC) boundary. It is thus of great interest both from physics and geophysics viewpoint to have a good understanding of the physical and chemistry properties of iron alloyed with Ni and other candidate light elements such as Si, O, and S in the solid and liquid states.

Measurements of physical properties of candidate iron alloys at the conditions of the OIC boundary, which is subject to 330 GPa and approximately 5500 K, are essentially needed to establish reliable physical constraints on the thermal and chemical states of the planet. Seismic observations of the Earth's outer and inner core, in particular, can be directly compared with experimental measurements of the acoustic sound velocity-density profiles of iron alloys at relevant P-T conditions, to derive the chemical compositional model of the core (Badro et al., 2006). Knowing the melting temperature and thermal transport properties (thermal conductivity and rheology) of iron alloys permits reliable evaluations of the heat transport (e.g., the amount of the latent heat), thermal evolution, and dynamic convection of the planet's deep layers.

Z can help: Making the aforementioned critical measurements experimentally has been very challenging due to the extreme P-T environments involved and intrinsic limitations in in-situ diagnostics of previously available dynamic and static techniques [e.g., Brown and McQueen, 1986; Nguyen and Holmes, 2004]. As such, deep-Earth scientists have relied on scaling laws and extrapolation of experimental data (e.g., Birch's Law, Wiedemann-Franz Law) to estimate the chemical composition and physical states of the planet's core [Birch, 1952], while our physical understanding of the cores of the exoplanets remains in uncharted territory as these planets were only discovered in recent years. The integration of the Z-Machine's extreme power, that can reach to very high pressures of hundreds of gigapascals while maintaining relatively low temperatures of thousands of degrees kelvin, with the optical and electronic diagnostics opens a new window to access the explored P-T regime using high-energy density techniques.

Melting Curve

Determination of the occurrence of melt will involve the combination of ellipsometry and VISAR measurements to sensitively determine changes in what physical properties across melting from solid to liquid iron. Since Si and Ni can readily alloy with Fe at ambient pressures and these alloys are also more readily available and can be fabricated relatively easily, our experimental efforts will start with pure iron and iron alloyed with 8wt% Si and approximately 5wt% Ni, and eventually move onto Fe with 8wt% S.

Previous studies have shown that the melting curve of iron determined from dynamic shock experiments is approximately 1000-2000 K higher than that extrapolated from static DAC experiments [e.g., Brown and McQueen, 1986; Tan and Ahrens, 1990; Shen et al., 1998; Nguyen and Holmes, 2004; Sola et al., 2009; Anzellini et al., 2014]. The discrepancy remains to be explained using future reliable experimental dynamic and static results. Kinetic barrier was used early on to explain this discrepancy in the measured melting temperatures, although recent static and dynamic measurements on other systems such as Ta agree with each other well. Our shock ramp experiments at isentropic conditions with sensitive diagnostics are thus ideally suited for studying the melting curves of iron and its alloys at high P-T where the melting curve tends to be flat. In support of this proposal, Lin's team will concurrently conduct high P-T DAC experiments using time-resolved laser heating and X-ray diffraction experiments at the Advanced Photon Source, Argonne National Laboratory to cross examine the melting curve of iron and its alloys at extreme conditions. Specifically, the team has recently used the diffused X-ray scattering signals using pulsed laser heating as a reliable means to detect melted iron alloy in a DAC.

Chemical Composition and Seismic Signatures of the Earth's Core

Recent seismic studies have revealed detailed signatures of the Earth's core including super-rotation, seismic anisotropy, and layering and heterogeneities of the inner core and "sedimentation" of the outermost outer core [e.g., Beghein and Trampert, 2003; Deuss et al., 2010; Belonoshko et al., 2007]. These observations indicate complex dynamic processes occurring during the formation of the inner core. These studies also provide reliable seismic velocity-density profiles of the region. Comparison of the seismic parameters of candidate iron alloys in the liquid and solid states with seismic profiles of the liquid outer core and solid inner core, respectively, thus provides first-order references to the physical and chemical states of the planet's interior. The velocity-density contrast across the melting of iron alloys at the inner-outer pressure of 330 GPa also provides an anchor point for the thermal-chemical states at the region that can be used to evaluate how much energy is released into the outer core to power the geodynamo. From this perspective, laboratory measurements on the velocity-density profiles and thermal EoS of candidate iron alloys at high P-T conditions are essential to resolve this key issue that is also related to the thermal chemical state of the whole Earth [e.g., Badro et al., 2006]. Indeed, there have been a plethora of static and dynamic high-pressure experiments as well as theoretical calculations conducted previously to tackle these issues. The major drawback, however, is that previous experiments have not been able to intercept realistic P-T conditions especially deep at the OIC boundary, because traditional shocks along the Hugoniot typically resulted melting of iron at approximately 200 GPa while producing high temperature in static high-pressure DAC experiments remains mostly challenging. The shock ramp applied by the Z-Machine, together with in situ diagnostics, allows direct probing of the acoustic and thermal transport properties of the iron alloys at much higher pressures relevant to the region while keeping the temperature relatively low.

Due to limited experimental results available, extrapolations and thermodynamic modelling have been used commonly to estimate the seismic profiles of iron alloys in the core and to deduce the chemical composition of the region. In particular, an empirical linear velocity-density relationship of iron alloys, Birch's Law, has been commonly used to extrapolate to inner core conditions without considering ultrahigh P-T effects, e.g., anharmonicity of iron alloys at extreme conditions especially in the liquid state [e.g., Badro et al., 2006; Lin et al., 2005; Mao et al., 2012]. It has been shown recently that high temperature can significantly decrease the compressional wave velocity (V_p) of the hcp-Fe and its alloys at a given density and that the V_p - ρ curve shows a concave behavior at the pressure regime of the Earth's core (Lin et al., 2005; Mao et al., 2012); that is, the high P-T effects on the velocity-density relationship can significantly affect our estimates of the amount of light elements and physical states of the Earth's core. A power-law function that accounts for both higher density and high-temperature effects has been reported to better describe the V_p - ρ relationship for hcp-Fe and hcp-Fe8wt%Si [Mao et al., 2012]. We should note that most of the previous studies mostly focus on the velocity-density relation of solid iron alloys, while the velocity-density behavior of the liquid iron and its alloy at relevant P-T condition of the planetary core remains largely lacking. This means many estimates based on a linear extrapolation of the sound velocity of solid iron alloys to higher density are likely imprecise or even incorrect.

Thus far, the thermal EoS and velocity-density profiles of iron and its alloys at pressures beyond approximately 250 GPa and high temperatures, especially at the conditions of the OIC boundary, remain mostly theoretical. Such theoretical calculations suffer from strong multi-electron correlations that are difficult to account for. Most importantly, there are only a handful of scattered results on the physical properties of liquid iron alloys at relevant OIC conditions, severely limiting our understanding of the chemical composition and geodynamo of the region. Experimental studies of the sound velocity at high P-T conditions especially into the liquid state, even as low as 100 GPa, will help to adjust these extrapolations as well as fundamental understanding of the fundamental EoS and acoustic wave physics of the most abundant transition metal in the planet. The Z-Machine's capability presents a unique opportunity to dissect the P-T space relevant to the Earth's core and exoplanets. The acquired thermal EoS and V_p - ρ data of iron and its alloys will be modelled using thermodynamics and finite-strain theory to construct a reliable velocity-density and EoS models to be compared with seismic profiles.

Thermal Evolutions and Dynamic State of the Planetary Cores

In the project, we will investigate the melting curve of Fe and the melting point depression of iron due to the light element alloying effect, such as the addition of Si, S, and O, at relevant P-T conditions of the outer-inner core (OIC) and exoplanets. The OIC not only defines the boundary between the solid inner core and liquid outer core as Earth is now, but also provides an anchor point for constraining temperature in the deep interior. Gradual cooling of the planet causes the OIC boundary to shift outward over time (i.e. inner core growth). Current estimates of the Earth's cooling rate suggest that the core began to crystallize about one billion years ago. Prior to this time the core would have been entirely liquid, so the power available to drive the geodynamo would have been different early in the Earth's evolution. Without the principal sources of buoyancy due to latent heat release and segregation of light elements into the liquid, the sole buoyancy source for driving convection is associated with cooling the liquid core. This mechanism is only viable if the cooling rate exceeds the rate the core would cool by thermal conduction if the fluid was well mixed (or isentropic). This is precisely why measurements of transport properties in liquid iron at high pressure and temperature are so important.

Recent theoretical calculations suggest that the thermal conductivity of liquid iron alloys is about a factor of two larger than previously thought [Pozzo et al., 2012, 2013; Zhang et al., 2015]. As a result, the cooling rate of the core needs to be higher to exceed the threshold for the onset of thermal convection, particularly before the formation of the inner core. Geological observations suggest that thermal convection did occur prior to the formation of the inner core because there is evidence for a magnetic field 3.5 billion years ago. On the other hand, models for the thermal evolution of the Earth imply that high heat flows are difficult to sustain over the age of the Earth. In other words, evidence for an ancient magnetic field seems to be incompatible with our current estimates for the transport properties of liquid iron alloys. Speculations that electron-electron scattering would substantially lower the thermal conductivity offer one possible resolution because these effects are not currently included in the predictions. The study of Zhang et al. [2015] suggest that these effects become important at high temperature, but it is not currently feasible to combine electron-phonon and electron-electron scattering into a single comprehensive calculations. Consequently, the proposed experiments have the potential to resolve an important question.

The proposed melting and conductivity measurements will provide *a number of key benchmarks for the first-principles simulations* performed in the group of collaborator Prof. Militzer of the UC Berkeley. Density functional molecular dynamics (DFT-MD) is the state-of-the-art simulation method of choice to study iron at high P-T conditions. While this method has been tested for many materials and conditions, it is not free of controlled and uncontrolled approximations. At the present time, very few benchmarks exist for hot, dense iron and it is thus unclear what the impact these approximations have. DFT-MD simulations are computationally demanding because iron has a large number of valence electrons that need to be treated explicitly (14 per atom), which has limited the size of almost all DFT-MD simulations to 64 atoms only. The error that is introduced by this size constraint has been difficult to assess because larger simulations are prohibitively expensive. In addition, DFT-MD relies on one uncontrolled approximation, the choice of the exchange-correlation functional that cannot be determined within the theory itself. The impact of this approximation has been difficult to quantify although Sola and Alfe (2009) derived a correction to the DFT-MD melting temperature of 500K by employing quantum Monte Carlo calculations. There is no experimental data available to verify that the 500K correction represents the right magnitude or even the correct sign. By providing benchmark results, we anticipate that the proposed melting measurements to improve the accuracy of first-principles simulations.

The proposed conductivity measurements would also contribute towards settling the current debate what is the correct value for iron's conductivity at high P-T and whether electron-electron scattering matters in addition to electron-phonon interactions. Only the latter is included in standard linear-response calculations that starting the DFT-MD trajectory and then applies the Kubo-Greenwood formula to a number of snapshots:

$$\sigma(k, \omega) = \frac{2\pi}{3\omega V} \sum_{i,j=1}^{\infty} \sum_{\nu=1}^3 \left[f(\epsilon_j^k) - f(\epsilon_i^k) \right] \left| \langle \psi_j^k | \nabla_{\nu} | \psi_i^k \rangle \right|^2 \delta(\epsilon_j^k - \epsilon_i^k - \hbar\omega) ,$$

where $\hbar\omega$ is the energy of the excitation, k is the wave vector, ψ are the Kohn-Sham single-particle wave functions, ϵ are the energy levels of each band, f is the Fermi-Dirac distribution, ∇ is the gradient-operator in direction ν , and V is the cell volume. Because one starts from single-particle wave function, no electron-electron scattering is included in this expression. However, this formula can be applied to the electronic contributions to the thermal and electric conductivity equally. Benchmarking one term would also shed light on the accuracy of theoretical predictions for the other.

This study additionally involves questions of a melting point depression and density contrast in the presence of light elements at the OIC [Li and Fei, 2003]. Planetary cores were likely formed during the early stage of the planetary formations when there were extensive collisions between smaller bodies that resulted extensive melting of the planet. As evidenced from geochemical and geophysical studies, the Fe-Ni that sank down to the core would contain certain amount of light elements—for the Earth’s core, it’s about 10wt% based on the density deficit between seismic profiles and mineral physics data, though the exact amount remains uncertain. As the planet evolved, heat was escaped from its core to the silicate mantle and an inner core is formed. Depending on the exact identity and amount of light elements in the iron alloys, the melting point depression can vary from approximately 500 K to perhaps 1000 K. The uncertainty in the melting point depression can translate to significant uncertainties in the evaluation of the outer core geotherm and the heat transfer across the core-mantle boundary [e.g., Buffett et al., 2002]. These scientific quests can be directly addressed using the experimental results from the Z-Machine by measuring the melting curves and thermal EoS of iron and its alight element alloys at relevant P-T conditions.

Physics and Chemistry of Exoplanets

The experimental results at extreme conditions that the Z-Machine can generate are also relevant to our understanding of the exoplanet evolution which remains largely unknown [Seager, 2010]. The discovery of these exoplanets raises a series of interesting questions including the possibility for planets that may sustain life and the presence of a magnetic field. In the interiors of these giant exoplanets, iron alloys are subject to even more extreme environments up to tens of Mbars where many questions about the thermal transport and EoS properties of a molten core are needed to be addressed using experimental results like the ones proposed here to have the first glimpse at the potential physical, chemical, and magnetic states of these planets. From measurements of the mass, radius and angular momentum information, theorists can posit the density distribution of planets, including the distribution of high-density materials, such as iron.

Similar challenges arise for the generation of magnetic fields in the interiors of super Earths. Theoretical estimates of thermal conductivity in iron are predicted to increase substantially with pressure, so very large thermal conductivities are expected in the cores of super Earths. The associated requirements on heat flow may be prohibitive, unless the effects of higher temperature can lower thermal conductivity. Experimental constraints on thermal conductivity at high pressure and temperature are essential for understanding the internal dynamics of rocky planets. Our proposed experiments could reach to 300 GPa and 5000 K conditions that corresponds to Earth-core conditions, but also corresponds to conditions at 0.75 Earth-radius depth of a super-Earth with 1.5 the radius of our Earth or 1.5 Earth-radius for a super-Earth with $\sim 2\times$ earth radius [Wagner et al., 2011; Seager et al., 2007].

Our measurements on the EoS, velocity-density profiles, and thermal transport properties of iron and its alloys will be used to build a velocity-density and thermodynamic model for understanding the density distribution and thermal transport states of these giant exoplanets. These results on the melting and conductivity of iron alloys in the liquid and solid phases will provide *a number of key benchmarks for the*

geodynamic simulations performed in the group of collaborator Prof. Buffett of the UC Berkeley. We will work with astrophysicists and geodynamicists to model potential dynamic convection patterns of a given exoplanet to test what are the physical and chemical conditions needed for a planet's core to evolve to produce a magnetic field and plate tectonic processes.

Competence and experience of key personnel

Tackling these key scientific quests requires an interdisciplinary approach involving expertise in physics, geophysics, geodynamics, and first-principles theory. The PIs have assembled a team of scientists and PhD graduate students for the research project. The research group of the Center for High Energy Density Science, along with Prof. Jung-Fu Lin's Mineral Physics Group, both at UT Austin (MRG), will team up with Sandia National Labs materials researchers to investigate the transport and acoustic properties and melting of iron alloys at extreme P-T. The proposed melting and conductivity measurements will also provide much needed benchmarks for first-principles computer simulations performed by Prof. B. Militzer of the University of California, Berkeley. In addition, Lin and Militzer's team will model the thermal equation of states and velocity profiles of iron and iron alloys using thermodynamics and finite-strain theory in order to make results easily accessible to a wide audience of scientists who work on matching seismic signatures with different chemical compositions of the Earth's core. PI Lin has been studying thermal elasticity and phase diagrams of iron alloys at static high P-T conditions in the last 15 years, and his team and collaborators will simultaneously conduct static DAC experiments coupled with synchrotron X-ray and laser spectroscopies and electrical conductivity techniques to measure velocities, phase diagrams, electrical and thermal conductivities of iron and its alloys at static high P-T to compare with the dynamic experimental results in order to satisfactorily model the physics and chemistry of the planetary core. Experimental melting curves of iron alloys available from these studies will allow scientists at UC Berkeley led by Prof. B. Buffett to evaluate the melting point depression due to the substitution of light element in the core and thus to derive the potential energy release through the crystallization of the solid inner core and the amount of energy contribution to the outer core geodynamo. Prof. Buffett's team at UC Berkeley will also use the thermal conductivity and melting curves of iron alloys to model geodynamic and geomagnetic evolution of the Earth's core as well as those of the exoplanets. These new experimental results will allow us to model physical and chemical states needed for an exoplanet to exhibit convection conditions for the generation of a magnetic field that may be needed to sustain life. These newly available experimental data will be integrated through interdisciplinary collaboration of the team scientists for a better understanding of the thermal and chemical states of terrestrial and exoplanetary cores.

PI Lin at the Department of the Geological Sciences and Texas Materials Institute:

PI Lin is a tenured faculty in the Department of Geological Sciences since 2008 and an adjunct faculty in the Texas Materials Institute since 2012. His research expertise focuses on studying mineral physics and condensed matter physics in extreme P-T environments using synchrotron x-ray and laser spectroscopic techniques in a DAC. PI Lin teaches Earth Materials, Optical Mineralogy, Mineral Physics, and Physics of the Earth courses at the Department that are of direct relevance to the proposed research. PI Lin and his research group investigate crystal structures, equation of states, elasticity, deformation and textures, and optical and transport properties of earth materials under extreme environments. They are also regular and partner users of various high-pressure synchrotron beamlines at the Advanced Photon Source (APS), and are well experienced with the application of the APS beamtimes, conduction of synchrotron experiments, and analyses of x-ray spectroscopic data (diffraction and imaging/tomography). PI Lin served as an APS Upgrade member as well as the General User Proposal (GUP) evaluation panel in recent years. PI Lin was a Lawrence Livermore Fellow (2005-2008) in the High Pressure Group of the Physics Directorate, and is knowledgeable with the dynamic compression of planetary materials. In recent years, PI Lin and his group have been involved in DOE and DOD related research projects including Energy Frontier Research in Extreme Environments (EFREE), High-Pressure Collaborative Access Team (HPCAT), the Carnegie-DOE Alliance Center of the National Nuclear Security Administration (NNSA), and Defense Threat Reduction Agency (DTRA). Dr Lin's group will analyze the results using thermal EoS and finite-strain

theory modelling, and will interrogate these dynamic measurements using comparison with static DAC experimental results.

PI Bernstein at the UT Center for High Energy Density Science:

Dr. Bernstein is Assistant Director of CHEDS since 2012. Prior to that, from 2006 to 2012, Aaron was Research Associate and Acting Deputy Director of the CHEDS. CHEDS is an Official Research Unit of the University, and an NNSA Center for Excellence for high-energy density science. CHEDS attracts excellent students to its program through its centerpiece laser, the Texas Petawatt Laser, which is among the highest power lasers in the world. During his time at CHEDS Aaron has participated in multiple single-shot materials dynamics experiments using lasers drivers (JANUS/LLNL, ZBL/Sandia, THOR and GHOST at CHEDS) to study spallation and damage of metals at high strain rates, concentrating on material strength dependence on grain size and material impurities. These experiments emphasized careful characterization of material composition and properties both before and after the experiment, elucidating the role of grain-size and inclusions on material strength and failure modes (brittle vs. ductile) at high strain rates, all relevant experience here. In his role as Assistant Director, he advises daily scientific activities of staff scientists, post-docs, and students at CHEDS. The ellipsometer proposed for use here is originally of Aaron's design, and he develops and maintains the collaborative project at Sandia to develop it for time-resolved single-shot measurements of the dielectric function of dynamic materials on Z.

Collaborating Partners at Sandia National Laboratory

The proposal leverages an ongoing experimental program with partners at Sandia National Laboratory, which uses gas-guns and VELOCE, an electromagnetic pulser at the DICE facility at Sandia National Labs. Sandia collaborators operate gas-guns at two facilities (STAR and DICE) that will be used to characterize initial target materials. Collaborator Dr. C. Seagle is a member of the Scientific Working Group that is committed to the long-term success of the Z Machine and is involved with the development of the shock ramp platform on the Z Machine. He will collaborate with the team on the design and analyses of the Z-Machine dynamic experiments. DR. Seagle led the experimental efforts to shock iron to a peak pressure of 280 GPa recently using the Z Machine. Dr. Seagle received his PhD in Geophysics from University of Chicago and is also an expert in geophysics of the deep Earth and physics of iron alloys in extreme environments. His expertise in geophysics will help the team to apply the experimental results to understand the geophysics and planetary science of iron cores. Dr. Dan Dolan has expertise fielding a gas gun at Brookhaven NSLS facility [Dolan, 2007]. Tom Ao, in particular, has expertise for producing specialized target designs that including bonding layers suitable for dynamic materials experiments [Ao et al., 2007].

Key Collaborators at University of California at Berkeley

Dr. Burkhard Militzer is a Professor in the Department of Earth and Planetary Science and is an expert in the theoretical calculations of planetary materials in extreme conditions of planetary interiors. He has developed theoretical models to simulate physical properties of materials in the rocky shells and liquid metal cores of terrestrial planets (e.g., Wahl and Militzer, 2015). He has been involved in NSF, DOE, and NNSA funded research projects relevant to condensed matter physics and warm dense matter physics in extreme pressures and temperatures.

Dr. Bruce Buffett is a Professor in the Department of Earth and Planetary Science and is an expert in the dynamics of planetary interior. He has developed numerical models to simulate convection and other dynamical processes in the rocky shells and liquid metal cores of terrestrial planets. He led the development of an open-source numerical geodynamo model called *Calypso*, which simulates convection and magnetic-field generation in the liquid metal. The code is designed for massively parallel computing and scales efficiently on 10^4 cores or more. This code will be used to assess the consequences of experimental results on magnetic-field generation in terrestrial planets.

Demands of the project in terms of resource requirements (AARON) 1.5 PAGES

Relevance and Outcomes/Impacts:

The proposed work will provide the first experimental constraints on electrical and thermal conductivity of liquid iron alloys at high P-T. Access to simultaneous high P-T will be essential to ascertain whether electron-electron scattering has an important role at high temperature and whether the electrical and thermal conductivity of liquid iron alloys will be within the range to sustain the generation of a magnetic field. These results will be used in numerical simulations of convection and magnetic-field generation to quantify the evolution of the magnetic field over geological time and to appraise the viability of field-generation in super Earths. These results will also help benchmark theoretical understanding of the fundamental physics including the contribution of the electron-electron scattering on the thermal transport properties of transition metal iron metal in the liquid and solid phase in extreme environments in the Earth's core and in super Earths. The proposed work will also provide experimental constraints on the melting curve of iron and melting point depression due to the substitution of a major light element at directly relevant conditions of the outer-inner core boundary. These results will impact our understanding of the thermal evolution and dynamics of the Earth's interior and super Earth.

Technical developments and scientific knowledge from studying classic transition metal iron alloys at extremes will be readily useful for future studies of other *d-f* alloys and compounds in extreme conditions using the Z-Machine. Specifically, we will develop sample designs and ellipsometer techniques readily available for future Z-Machine users interested in using them. The use of these techniques on other *d-f* metals and compounds will have direct relevance to the national security and materials understanding.

Project Management Plan (Appendix):

This section should identify the activities/tasks to be performed, a time schedule for the accomplishment of the activities/tasks, and the expected dates for the release of outcomes. Applicants may use their own project management system to provide this information. This plan should identify any decision points and go/no-go decision criteria. Successful applicants must use this project timetable format to report progress variances. Please provide the Project Management Plan as an appendix to your Project Narrative. This appendix will not count in the Project Narrative page limitation.

To be shown in Gantt chart form, then described:

[As preparation for the proposed shots, we will perform ellipsometry on shock or shock-ramp experiments that release into LiF, as ridealong shots in late Summer of 2016. We will perform the proposed experiments on a variety of target types at earth-core relevant conditions on the interrogation plane. These will have some fraction of shots using ellipsometry, with a major decision point before the proposed shots, based on the ride-along shots. Because a mapping of acoustic velocity along P-T is interesting for a variety of the materials, we will elect P-T accordingly. We will then perform a down-select of interesting target types, conditions, and diagnostics. This decision point will consider the choice between concentrating on the melting curve of iron, filling in the velocity vs. P-T parameter space, or exploring iron conductivity over a range of particularly relevant conditions.]

So, ridealong shots, decide on diagnostics, then proposed shots, then sample down select, then final proposed shots. During ridealongs, we will conduct further ellipsometry experiments on gas guns and Sean will do simulations based on Laslo. The planetary scientists will inform on sample selection and (with results of Sean's simulation) inform on sample design for first proposed Z shots. Planetary scientists will evaluate the usefulness of the data resulting from the first set of Z shots, and help decide on a down-select of possible samples in the second round of proposed shots.]

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Facilities and Other Resources (Appendix):

PI Bernstein at Department of Physics, UT Austin

Aaron Bernstein has been collaborating with Sandia for a few years on the development of the ellipsometer. As such, we have a well-defined set of resources available for this project, which we will continue to use for the proposed work. There are resources available for this research at the University of Texas. This includes a machine-shop in-house of the Physics Department and various semi-conductor fabrication facilities and relevant diagnostics. Facilities we have access to include: (1) UT-Austin Center for Nano- and Molecular Science (2) the Microelectronics Research Center, and in the UT Physics department (3) cryoshop (metal deposition capabilities) (4) machine shop. We also have access as part of Aaron's affiliation with the department to multiple optical laboratories and diagnostics equipment.

Of note, ellipsometer development will continue throughout this proposal, using the DICE facility at Sandia.

The DICE facility at Sandia consists of an optics lab, target fabrication, a gas gun, and a pulsed power machine. The optics lab is used for staging and development. We do testing and initial setup of our ellipsometry diagnostic here, where we have access to an optical table, oscilloscopes, lasers, and detectors. There are target fabrication and machining facilities operated by the DICE facility members. This is where many parts for shots are made and assembled, including projectiles, target plates, and occasionally the samples themselves. The gas gun is capable of launching projectiles up to about 300 m/s, and can accommodate a heated projectile, up to 300 degrees Celsius. Standard diagnostics include PDV and point VISAR. The pulsed machine is capable of reaching pressures approaching 10 GPa.

UT student Sean Grant has become facile in the use of Laslo for conducting simulations relevant to the design of targets and Z-machine configuration for this project. This includes use of Laslo on the following machines:

Red Sky: 264 Tflops, 2,846 nodes (22,768 cores)

Glory: 38 Tflops, 272 nodes (4,352 cores)

Sky Bridge: 600 Tflops, 1848 nodes (29,568 cores)

Further, Sandia has supported this project with engineering support, made available to assist in the designing of parts. There is also a Z facility crew that generally handles target fabrication, capable of continued fabrication of pure-iron targets.

PI Lin at Department of the Geological Sciences and Texas Materials Institute, UT Austin

The PI's Mineral Physics laboratory has a variety of diamond cells and an inventory of diamonds for the complimentary static experiments in extreme environments. These will be interfaced with the synchrotron X-ray and laser optical spectroscopic systems for high pressure-temperature research. The PI's Laboratory is also equipped with an optical Raman system, a high-pressure gas loading system, and a sample preparation lab to prepare various samples for the proposed research. The Department of Geological Sciences at the Jackson School of Geosciences houses a machine shop with a full-time machinist. The Texas Materials Institute, Nano Center, and Department of Geological Sciences have a variety of facilities available for sample synthesis and characterization including TEM/STEM, SEM, XRD, and FIB. PI Lin holds a joint faculty appointment at the Texas Materials Institute, and he and his associates have full access to using these analytical facilities.

Lin Mineral Physics Laboratory

Diamond anvil cells (symmetric, 2/3-fold panoramic, and short symmetric)

High-Pressure Gas Loading System (for loading gases such as He, Ne, Ar)

Sample Preparation Lab

Department of Geological Sciences

Machine and electronic shops, X-ray diffractometer for powder diffraction, Electron Microprobe (EPMA; JEOL 8200), Scanning Electron Microscope (SEM; JEOL T330A)

Texas Materials Institute (PI Lin is an affiliated faculty at the Institute)

Four-probe resistivity, thermal conductivity and thermoelectric power; Four-circle single crystal diffractometer

Center for Nano- and Molecular Science at TMI

Transmission Electron Microscope (JEOL 2010F; FEI TECHNAI G2 F20), SEM/STEM (Hitachi S-5500), SEM/FIB (FEI Strata DB235 with Zyvex S100)

Aerospace Engineering Department

Machine and electronic shop

Texas Advanced Computing Center

User-based computational user community access to petascale computing systems, remote and collaborative visualization resources, high-performance local disk file systems, and a petascale data archive. UT faculty and collaborators have on-campus research privilege to access the facility.

Experimental Requirements (Appendix):

This section should contain information on the technical requirements necessary to complete a successful experiment. Please provide the Z facilities detailed information as an appendix to your Project Narrative.

This appendix (Appendix A of this document) will not count in the Project Narrative page limitation.

Diagnostics requirements, including both standard and new diagnostics.

Machine configuration, including: Marx charge voltage, desired current, pulse length, prepulse suppression, and estimated pulse shape.

Load & Target hardware requirements (include diagram of target concepts/PowerPoint or scanned hand-drawn sketch is acceptable.)

Environment, Safety, and Health Hazards such as beryllium, lithium, heavy metals, gases, explosives, etc. Safety is of utmost importance at the Z facility; please describe any material or process that can pose a hazard to the operations staff or the facility.

Roles of Collaborators/Participants (Appendix):

PI Bernstein at UT Austin: XXX

PI Lin at UT Austin: PI Lin will coordinate experimental and theoretical research efforts and geophysical/planetary implications. PI Lin and his collaborators at UT Berkeley will integrate these newly available experimental data through interdisciplinary collaboration of the team scientists for a better understanding of the thermal and chemical states of terrestrial and exoplanetary cores. PI Lin and Militzer's team will model the thermal equation of states and velocity profiles of iron and iron alloys using thermodynamics and finite-strain theory in order to make results easily accessible to a wide audience of scientists who work on matching seismic signatures with different chemical compositions of the Earth's core. PI Lin will simultaneously conduct static DAC experiments coupled with synchrotron X-ray and laser spectroscopies and electrical conductivity techniques to measure velocities, phase diagrams, electrical and thermal conductivities of iron and its alloys at static high P-T to compare with the dynamic experimental results in order to satisfactorily model the physics and chemistry of the planetary core.

Prof. Militzer at UC Berkeley: Prof. Militzer's group will perform theoretical calculations to understand the thermal transport properties and melting curves of iron alloys at relevant P-T conditions of the Earth's core and that of super Earth. He will use the experimental results to benchmark theoretically calculated values on thermal conductivity and melting curve in order to understand the roles of high pressure, high temperature, and substitution of an alloying light element on the physics of liquid iron at extreme conditions. He will also team up with Lin's team at UT Austin to model the experimental results using thermal EoS and finite-strain theory.

Prof. Buffett at UC Berkeley: Experimental melting curves of iron alloys available from these studies will allow scientists at UC Berkeley led by Prof. B. Buffett to evaluate the melting point depression due to the substitution of light element in the core and thus to derive the potential energy release through the crystallization of the solid inner core and the amount of energy contribution to the outer core geodynamo. Prof. Buffett's team at UC Berkeley will also use the thermal conductivity and melting curves of iron alloys to model geodynamic and geomagnetic evolution of the Earth's core as well as those of the exoplanets. These new experimental results will allow us to model physical and chemical states needed for an exoplanet to exhibit convection conditions for the generation of a magnetic field that may be needed to sustain life.

Evaluation Phase (Appendix): (Aaron)

This section must include a plan and metrics to be used to assess the success of the project. Please provide the Evaluation Phase information as an appendix to your Project Narrative. This appendix will not count in the Project Narrative page limitation.

Biographical Sketch Appendix: Jung-Fu Lin

Affiliation and Address

Department of Geological Sciences, Jackson School of Geosciences
The University of Texas at Austin, 1 University Station C1100, Austin, TX 78712
Phone: 512-471-8054, Fax: 512-471-9425 Email: afu@jsg.utexas.edu

a. Education and Training

National Cheng-Kung University	Earth Sciences	B.S., 1992
National Cheng-Kung University	Earth Sciences	M.S., 1994
The University of Chicago	Geophysics	Ph.D., 2002

b. Research and Professional Experiences

2012-current Associate Professor, The University of Texas at Austin
2008-2012 Assistant Professor, The University of Texas at Austin
2005-2008 Lawrence Livermore Fellow, Lawrence Livermore National Laboratory
2003-2005 Research Scientist, CDAC, Geophysical Laboratory, Carnegie Institution
2002-2003 Carnegie Postdoc Fellow, Geophysical Laboratory, Carnegie Institution

c. Ten Relevant Representative Publications:

Nayak, A. P., Z. Yuan, B. Cao, J. Liu, J. Wu, S. T. Moran, T. Li, D. Akinwande, C. Jin, **J. F. Lin**, Pressure-Modulated Conductivity, Carrier Density, and Mobility of Multilayered Tungsten Disulfide, *ACS Nano*, DOI: 10.1021/acsnano.5b03295, 2015.

Goncharov, A. F., S. S. Lobanov, X. Tan, Gregory T. Hohensee, D. G. Cahill, **J. F. Lin**, S.-M. Thomas, T. Okuchi, and N. Tomioka, Experimental study of thermal conductivity at high pressures: implications for the Deep Earth's interior, *Phys. Earth Planet. Inter.*, <http://dx.doi.org/10.1016/j.pepi.2015.02.004>, 2015.

Liu, J., **J. F. Lin**, A. Alatas, and W. Bi, Sound velocities of bcc-Fe and Fe_{0.85}Si_{0.15} alloy at high pressure and temperature, *Phys. Earth Planet. Inter.*, 233, 24-32, 2014.

Lin, J.F., S. Speziale, Z. Mao, and H. Marquardt (2013), Effects of the electronic spin transitions of iron in lower-mantle minerals: implications to deep-mantle geophysics and geochemistry. *Rev. Geophys.*, 51, 244-275.

Hunter, L.R., J.E. Gordon, S. Peck, D. Ang, and **J.F. Lin** (2013), Using the Earth as a Polarized Electron Source to Search for Long-Range Spin-Spin Interactions, *Science*, 339, 928-932.

Mao, Z., **J. F. Lin**, J. Liu, A. Alatas, L. Gao, J. Zhao, and H. K. Mao, Sound velocities of Fe and Fe-Si alloys in the Earth's core, *Proc. Natl. Acad. Sci.*, 109, 10239-10244, 2012.

Lin, J.F., H. P. Scott, R. A. Fischer, Y.-Y. Chang, I. Kantor, and V. B. Prakapenka, Phase relations of Fe-Si alloy in Earth's core, *Geophys. Res. Lett.*, 36, L06306, 2009.

Lin, J.F., G. Vankó, S.D. Jacobsen, V. Iota-Herbei, V.V. Struzhkin, V.B. Prakapenka, A. Kuznetsov, and C.S. Yoo (2007), Spin transition zone in Earth's lower mantle, *Science*, 317, 1740-1743.

Lin, J.F., V. V. Struzhkin, S. D. Jacobsen, M. Hu, P. Chow, J. Kung, H. Liu, H. K. Mao, and R. J. Hemley (2005), Spin transition of iron in magnesiowüstite in Earth's lower mantle, *Nature*, 436, 377-380.

Lin, J.F., W. Sturhahn, J. Zhao, G. Shen, H. K. Mao, and R. J. Hemley, Sound velocities of hot dense iron: Birch's law revisited, *Science*, 308, 1892-1894, 2005.

d. Synergistic Activities

2015-current Editorial Board, Nature Scientific Reports
2012-2015 Facilities Committee Member, COMPRES
2011-current Lecturer for UTeach Outreach Program at University of Texas at Austin
2012-current Visiting Professorship, Okayama University at Misasa, Japan
2009-2014 Academic Partner of the EFree Center of the EFRCs

e. Collaborators and Other Affiliations

UT Austin Collaborators

Steve Grand (Professor in Geological Sciences; Deep-Earth geophysics, NSF Frontier in Earth System Dynamics), James Gardner (Professor in Geological Sciences; Acquisition of piston-cylinder apparatus from NSF Instrumentation and Facility, Deep carbon observatory), Danny Stockli/Adam Goldsmith (Professor/PhD student in Geological Sciences; Raman study of radiation-damaged zircon), Elaine Li (Assistant Professor in Department of Physics; Brillouin light scattering and ultrafast laser spectroscopy), Jianshi Zhou (Research Professor in Department of Mechanical Engineering; properties of superconductors using X-ray and neutron diffraction), Todd Ditmire (Associate Director in Department of Physics; co-PI for Center for High Energy Science funded by DOE), Aaron Bernstein (Associate Director in Department of Physics; shock wave experiments on iron alloys at Sandia National Lab), Jinguang Cheng (Postdoc Research Fellow in Department of Mechanical Engineering; material science research at high pressures), Avinash Nayak (PhD student) and Deji Akinwande (Professor) at the Department of Electrical Engineering.

Collaborators at Other Affiliations

Ercan E. Alp (Argonne National Lab), Paul Chow (Carnegie Institution), Tom Duffy (Princeton University), Przemek Dera (University of Chicago), Leonid Dubrovinsky (Universität Bayreuth), Alexander G. Gavriluk (Russian Academy of Sciences), Alex Goncharov (Carnegie Institution), Steven Jacobsen (Northwestern University), Jennifer Jackson (California Institute of Technology), Ignace Jarrige (SPRING-8), Changqing Jin (Chinese Academy of Sciences), Michael Lerche (Argonne National Lab), Igor Lyubutin and S. G. Ovchinnikov (Russian Academy of Sciences), Takuo Okuchi (Okayama University), Vitali Prakapenka (University of Chicago), Henry Scott (University of Indiana-South Bend), Sergio Speziale (GeoForschungsZentrum Potsdam), Viktor Struzhkin (Carnegie Institution), György Vankó (KFKI, Hungary), Taku Tsuchiya (Ehime University), Heather Watson (Northern Illinois University), Rudy Wenk (University of California at Berkeley), Yuming Xiao (Carnegie Institution), Wenge Yang (HPSync, Argonne National Lab), Jiyong Zhao (Argonne National Lab)

PhD advisors: D. Heinz (University of Chicago)

Postdoc advisors: H.K. Mao & R.J. Hemley (Geophysical Lab)

Thesis Advisee and Postgraduate-Scholar Sponsor (*in last five years*)

Graduate students: S. Fu (UT Austin), J. Liu (UT Austin), C. Lu (UT Austin), J. Yang (UT Austin), X. Tong (UT Austin), Avinash Nayak (UT Austin)

Postdoc Researchers: Junjie Wu (Chinese Academy of Science), Z. Mao (University of Science and Technology in China)

Grad Students: 4

Post Docs: 2

Biographical Sketch Appendix: Aaron Bernstein

Affiliation and Address

Department of Physics, The University of Texas at Austin
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Biographical Sketch Appendix: Burkhard Militzer

Associate Professor, Department of Earth and Planetary Science,
Department of Astronomy, University of California, Berkeley
Email: militzer@berkeley.edu, Web: <http://militzer.berkeley.edu>
Phone: (510) 643-7414, Fax: (510) 643-9980

Education and Training:

2000-2003 Postdoctoral scientist, Lawrence Livermore National Laboratory
1996-2000 University of Illinois at Urbana-Champaign, Ph.D. in physics
1990-1996 Humboldt University, Berlin, Germany, diploma in physics
1992-1993 University of Oxford, UK

Research and Professional Experiences:

2011-present Associate Professor, Department of Earth and Planetary Science and
Department of Astronomy, University of California, Berkeley
2007-2011 Assistant Professor, University of California, Berkeley
2003-2007 Associate staff member, Carnegie Institution of Washington

PRODUCTS RELATED TO PROJECT:

- (1) S. Wahl, B. Militzer, "High-temperature miscibility of iron and rock during terrestrial planet formation", *Earth and Planetary Science Letters* **410** (2015) 25.
- (2) S. M. Wahl, H. F. Wilson, B. Militzer, "Solubility of iron in metallic hydrogen and stability of dense cores in giant planets", *Astrophysical Journal* **773** (2013) 95
- (3) H. F. Wilson, B. Militzer, "Rocky core solubility in Jupiter and giant exoplanets", *Phys. Rev. Lett.* **108** (2012) 111101. Suggested read by PRL editor.
- (4) B. Militzer, W. B. Hubbard, "Ab Initio Equation of State for Hydrogen-Helium Mixtures with Recalibration of the Giant-Planet Mass-Radius Relation", *Astrophysical Journal* **774** (2013) 148
- (5) K. P. Driver, B. Militzer, "All-Electron Path Integral Monte Carlo Simulations of Warm Dense Matter: Application to Water and Carbon Plasmas", *Phys. Rev. Lett.* **108** (2012) 115502.

OTHER SIGNIFICANT PRODUCTS:

- (1) H. F. Wilson, M. L. Wong, B. Militzer, "Superionic to superionic phase change in water: consequences for the interiors of Uranus and Neptune", *Phys. Rev. Lett.* **110** (2013) 151102
- (2) H. W. Wilson, B. Militzer, "Sequestration of noble gases in giant planet interiors", *Phys. Rev. Lett.* **104** (2010) 121101, selected for commentary by J. Fortney "Peering into Jupiter" in *Physics* **3** (2010) 26.
- (3) B. Militzer, "First Principles Calculations of Shock Compressed Fluid Helium", *Phys. Rev. Lett.* **97** (2006) 175501.
- (4) S. X. Hu, B. Militzer, V. N. Goncharov, S. Skupsky, "Strong-Coupling and Degeneracy Effects in Inertial Confinement Fusion Implosions", *Phys. Rev. Lett.* **104** (2010) 235003.
- (5) B. Militzer, D. M. Ceperley, "Path Integral Monte Carlo Calculation of the Deuterium Hugoniot", *Phys. Rev. Lett.* **85** (2000) 1890.

SYNERGETIC ACTIVITIES:

- Co-Organizer of program on "Dynamics and Evolution of Earth-like Planets" at the Kavli Institute for Theoretical Physics, Santa Barbara, Jan. 20 – Mar. 26, 2015.
- Organization of two NSF-funded summer schools in Urbana, IL, 2007 and 2012 with respectively 60 and 45 participating students and postdocs. Given lectures and hands-on computer labs.
- Referee for journals *Physical Review Letters*, *Physical Review A* and *B*, *Science*, *Nature Communications*, *Physics of the Earth and Planetary Interiors*, etc.

- Organization of computational Mineral and Rock Physics sessions at series of American Geophysical Union meetings; special session on Earth and Planetary Materials at the March meeting of American Physical Society, 2005.
- Participation in conference calls and workshops in Lawrence Livermore National Laboratory's collaboration with universities to use the National Ignition Facility for planetary science applications.

HONORS:

1996-1997 Scholarship from the German Academic Exchange Service (DAAD)

PROFESSIONAL MEMBERSHIPS:

American Physical Society, American Geophysical Union

COLLABORATORS AND OTHER AFFILIATIONS:

Collaborators: L. Bildsten, F. Brügge, S. A. Bonev, R. E. Cohen, L. A. Collins, K. Driver, J. Fortney, A. Goncharov, V. N. Goncharov, E. Gregoryanz, R. J. Hemley, R. Hennig, W. B. Hubbard, E. Huff, T. Hurford, J. D. Johnson, J. Kim, W. Kraft, J. D. Kress, X. Y. Li, J.-F. Lin, P. Lopez Rios, M. Manga, H.-k. Mao, L. Mitás, S. Mazevet, R. J. Needs, E. L. Pollock, M. A. Richards, B. Romanowicz, S. Seager, M. F. Stallmann, D. J. Stevenson, V. V. Struzhkin, S. Skupsky, E. de Sturler, M. D. Towler, C. Umrigar, H.-R. Wenk, J. W. Wilkins, Z. Wu

Graduate Advisors and Postdoctoral Sponsors: W. Ebeling, D.M. Ceperley, G. Galli.

Students supervised: R.L. Graham, F. Gonzalez, S. Jacobsen, D. O'Kane, J. Prancevic, A. Rhoden, G. Shi, I. Tamblyn, J. Tollefson, S. Wahl, M. Wong, S. Zhang

Postdocs supervised: K. P. Driver, K. P. Esler, S. Khairallah, S. Stackhouse, J. Vorberger, H. F. Wilson.

Co-investigators: D. M. Ceperley, E. de Sturler, J. Du Bois, R. E. Cohen, A. McNamarra, B. Romanowicz, E. R. Schwegler, H.-R. Wenk

Biographical Sketch Appendix: Bruce Buffett

Present Position: Professor
Campus Address: Department of Earth & Planetary Science
University of California, Berkeley
Berkeley, CA 94720
email: bbuett@berkeley.edu

Education and Training

Ph.D. Geophysics, Harvard University, 1991
M.Sc. University of Calgary, 1985
B.Sc. University of Toronto, 1981

Research and Professional Experiences

Professor, University of California, 2008-
Professor, University of Chicago, 2003-2008
Visiting Professor, UC Berkeley, 2000 (Spring Term)
Visiting Professor, Harvard University, 1999 (Fall Term)
Associate Professor, University of British Columbia, 1998 {2002
Assistant Professor, University of British Columbia, 1993 {1998.
Research Fellow, Institute of Theoretical Geophysics, University of Cambridge, 1991 {1992.
Research Assistant, Harvard-Smithsonian Center for Astrophysics, 1985 {1986.

Awards

Elected Associate of the International Association of Geodesy, 1993
Killam Faculty Research Fellowship, 1999
Graduate Teaching Prize, University of British Columbia, 1999
Fellow of American Geophysical Union, 2005

Five Relevant Papers:

Buffett, B.A., Geomagnetic fluctuations reveal stable stratification at the top of the Earth's core, *Nature*, 507, 484-487 (2014).
Matsui, H., King, E., and B.A. Buffett, Multiscale convection in a geodynamo simulation with uniform heat flux along the outer boundary, *Geochem. Geophys. Geosys.*, 15(8), 312-3225, (2014).
Buffett, B.A., Tidal dissipation and the strength of the Earth's internal magnetic field, *Nature*, 468, 952-954 (2010).
Buffett, B.A. and C.T. Seagle, Stratification at the top of the core due to chemical interactions with the mantle, *J. Geophys. Res.*, 115, B04407 (2010).
Buffett, B.A., The thermal state of Earth's core, *Science*, 299, 1675-1677 (2003).

Five Other Papers:

Buffett, B.A. and H. Matsui, Fluid dynamics of inner-core growth, *Phys. Earth Planet. Inter.*, 243, 22-29, (2015).
Buffett, B.A. and T.W. Becker, Bending stress and dissipation in subducted lithosphere, *J. Geophys. Res.*, 117, B05413 (2012).
Buffett, B.A., Onset and orientation of convection in the inner core, *Geophys. J. Int.*, 179, 711-719 (2009).
Buffett, B.A., A bound on heat flow below a double crossing of the perovskite – postperovskite phase transition, *Geophys. Res. Lett.*, 34, L17302 (2007).
Buffett, B.A., Estimates of heat flow in the deep mantle based on the power requirements for the geodynamo, *Geophys. Res. Lett.*, 29(12), doi: 10.1029/2001GL014649 (2002).

Synergistic Activities

Editor, Earth & Planetary Science Letters, 2015-present
Chair, AGU Committee for Studies of Earth's Deep Interior, 1998-2000
President, SEDI (a Union Committee of IUGG), 2003-2007
Advisory Board, COMPRES, 2003-2006
Faculty Instructor in Geodynamics, CIDER, UC Santa Barbara, 2004, 2008, 2012, 2014

Collaborators (past 48 months)

David Archer (U. Chicago), Thorsten Becker (USC), Ed Garnero (Arizona State), Gary Glatzmaier (UC Santa Cruz), Tom Herring (MIT), Raymond Jeanloz (UC Berkeley), John Lister (U. Cambridge), Sonny Matthews (Smithsonian Astrophys. Obs.), Paul Roberts (UCLA), Rudy Wenk (UC Berkeley); Co-Editors (past 24 months) Alan Beck (U. Western Ont.), Russ Evans (Brit. Geol. Sur.), Martyn Unsworth (U. Alberta), Steven Ward (UCSC)

Graduate Students & Postdocs (M.Sc and Ph.D)

Alan Rempel (M.Sc. 93-95, U Oregon), Julian Douglass (M.Sc. 93-95), David McMillan (M.Sc. 94-96, York U.), Kevin Kingdon (M.Sc. 95-98, GIF Inc.), Mathieu Dumberry (M.Sc., 95-98, U. Leeds), Olga Zatsepina (Ph.D. 94-99; PDF 99-02, U. Calgary) Simona Costin (M.Sc. 99-02, U. Sask), Matthew Davie (M.Sc. 00-02, Exxon), Jon Mound (PDF 01-02, U. Leeds), Hiroaki Matsui (PDF 03-pres, UCB), Chris Scullard (Ph.D 04-08, LLNL), Emily O'Donnell (Ph.D 04-08., U. Chicago), Ian Rose (Ph.D. 09-pres.), Jennifer Frederick (Ph.D 10-15.)
Eric King (PDF 10-pres.), Nick Knezek (PhD 14-pres.)
Total of 12 graduate students and 4 postdocs (currently 2 grad. students and 2 postdoc.)

Supervisors

Doctoral - Irwin Shapiro (Director, Harvard-Smithsonian Center for Astrophysics)
Postdoctoral - Herbert Huppert (Director, Institute for Theoretical Geophysics)

Sandia National Laboratories Z facilities will provide:

- 4 shot weeks (approx.. 20 shots) in CY 2016 and 2017 from April 1, 2016 to December 31, 2017.
- Experimental time, 3 to 5 shots per calendar year range.
- Basic power feed hardware
- Standard diagnostics
- Load assemblies and most targets

Current and Pending Support: Jung-Fu Lin

1. Project/Proposal Title: Career: Phase Diagrams and Elasticity of Iron Alloys in the Earth's Core

Source of Support: NSF Career EAR-1056670

Total Award Amount: \$542,898

Total Award Period Covered: 1/1/2011-12/31/2015 (Current)

PI: Jung-Fu Lin

2. Project/Proposal Title: Physics and Chemistry of Carbon at Extreme Conditions

Source of Support: Sloan Foundation (Deep Carbon Observatory)

Total Award Amount: \$56,000

Total Award Period Covered: 10/1/2013-9/30/2015 (Current)

PI: Jung-Fu Lin (UT Austin as a partner)

3. Project/Proposal Title: Elasticity and Spin Transitions of Iron in the Earth's Lower Mantle

Source of Support: NSF Geophysics

Total Award Amount: \$361,149

Total Award Period Covered: 1/1/2015-12/31/2017 (Current)

PI: Jung-Fu Lin

4. Project/Proposal Title: Collaborative project: CSEDI- Understanding Si and Fe differentiation in Earth's mantle and core through experimental and theoretical research in geochemistry and mineral physics

Source of Support: NSF CSEDI

Total Award Amount: \$226,275

Total Award Period Covered: 4/1/2015-3/30/2018 (Current)

PIs: Nicolas Dauphas (U Chicago), Jung-Fu Lin (UT Austin), Renata Wentzcovitch (U Minnesota)

5. Project/Proposal Title: Properties of Transition Metals under Extreme Conditions

Source of Support: Stewardship Science Academic Alliances, Department of Energy

Total Award Amount: \$900,000

Total Award Period Covered: 06/01/2015-05/31/2018 (Pending)

PIs: Jung-Fu Lin (lead PI), Alexander Goncharov (Carnegie Institution)

6. Project/Proposal Title: Understanding Macroscopic and Microscopic Behaviors of Shocked Crustal Materials through Dynamic Imaging and Diffraction

Source of Support: Department of Defense

Total Award Amount: \$750,000

Total Award Period Covered: 08/01/2014-07/31/2017 (Pending)

PIs: Jung-Fu Lin, Aaron Bernstein (UT Austin)

Current and Pending Support: Aaron Bernstein

1. **Project/Proposal Title:** Understanding Macroscopic and Microscopic Behaviors of Shocked Crustal Materials through Dynamic Imaging and Diffraction

Source of Support: Department of Defense

Total Award Amount: \$750,000

Total Award Period Covered: 08/01/2014-07/31/2017 (Pending)

PIs: Jung-Fu Lin, Aaron Bernstein (UT Austin)

Current and Pending Support: Burkhard Militzer

Title: Path Integral Monte Carlo Simulations of Dense Plasmas with Heavier Elements

Agency: NSF/DOE Partnership in Basic Plasma Science and Engineering

PI: Burkhard Militzer

Period: 07/01/2013 to 06/31/2016 Amount: \$690,000.

BM's commitment: 0.50 summer months per year Location: UC Berkeley

Title: Computational Modeling of Interiors of Sub-Neptunes and Gas Giant Planets

Agency: National Science Foundation, Astronomy and Astrophysics Research Grants

PI: Burkhard Militzer

Period: 08/01/2014 to 07/31/2017 Amount: \$369,548.

BM's commitment: 1.00 summer months per year Location: UC Berkeley

Title: CSEDI Collaborative Research: A Multidisciplinary Approach to Investigate the Origin of Anisotropy at the Base of the Mantle"

Agency: National Science Foundation, CSEDI program

PIs: Barbara Ramonowicz, Hans-Rudolf Wenk, Allen McNamara, Burkhard Militzer

Period: 07/01/2015 to 06/30/2018 Amount at UCB: \$411,355 (Pending)

BM's commitment: 0.00 summer month pers year Location: UC Berkeley and UC Santa Cruz

Title: Saturn's Interior at Cassini Solstice"

Agency: NASA CDAPS15 Program

PIs: Jonathan Fortney, Burkhard Militzer

Period: 04/01/2016 to 03/31/2019 Amount at UCB: \$261,151 ((Pending)

BM's commitment: 0.00 summer month pers year Location: UC Santa Cruz and UC Berkeley

Current and Pending Support: Bruce Buffett

Title: Integrating models of mantle convection and true polar wander, and the structure of the Earth's deep interior

Agency: NSF

PI: Bruce Buffett

Period: 01/01/2013 to 12/31/2015 Amount: \$214,530.

Title: FESD Proposal Type II: CIDER-II Synthesis Center: Cooperative
Institute for Dynamic Earth Research (co-PI)

Agency: National Science Foundation, Astronomy and Astrophysics Research Grants

Co-PI: Bruce Buffett

Period: 10/01/2011 to 09/30/2016 Amount: \$2,532,931.

Title: Geomagnetic signals from the Earth's core: Searching for evidence of waves and stable stratification

Agency: National Science Foundation

PI: Bruce Buffett

Period: 07/01/2014 to 06/30/2017 Amount: \$227513 (Pending)

Appendix

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND No. 2015-XXXX